

n-Hexane  
110-54-3 | DTXSID0021917

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

## Model Results

**Predicted value:** 3.96

**Global applicability domain:** Inside

**Local applicability domain index:** 6.80e-01

**Confidence level:** 7.87e-01

## Nearest Neighbors from the Training Set

Image not found

n-Hexane

**Measured:** 3.90

**Predicted:** 3.96

Image not found

Heptane

**Measured:** 4.66

**Predicted:** 4.56

Image not found

Pentane

**Measured:** 3.39

**Predicted:** 3.15

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(2E)-2-Octene

**Measured:** 4.51

**Predicted:** 4.48

Image not found

3-Methylpentane

**Measured:** 3.60

**Predicted:** 3.59